

# Threshold singularities in the dynamic response of gapless integrable models

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We develop a method of an asymptotically exact treatment of threshold singularities in dynamic response functions of gapless integrable models. The method utilizes the integrability to recast the original problem in terms of the low-energy properties of a certain deformed Hamiltonian. The deformed Hamiltonian is local, hence it can be analysed using the conventional field theory methods. We apply the technique to spinless fermions on a lattice with nearest-neighbors repulsion, and evaluate the exponent characterizing the threshold singularity in the dynamic structure factor.

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One-dimensional (1D) interacting systems [1, 2, 3] occupy a special place in quantum physics. Although interactions have much stronger effect in 1D than in higher dimensions, it is often possible to evaluate observable quantities exactly. Besides forming the basis of our understanding of strong correlations, 1D models have long served as a test bed for various approximate methods.

Many properties of interacting 1D systems can be understood by considering integrable models [2]. The paradigmatic example is  $N$  spinless fermions on a lattice with  $L$  sites with periodic boundary conditions,

$$H = \sum_{m=1}^L \left[ -\psi_m^\dagger \psi_{m+1} - \psi_{m+1}^\dagger \psi_m + 2\Delta n_m n_{m+1} \right]. \quad (1)$$

Here  $n_m = \psi_m^\dagger \psi_m$  and  $\Delta$  is the repulsion strength [4]. The experimentally relevant [5] response function for the model (1) is the dynamic structure factor

$$S(q, \omega) = \frac{2\pi}{L} \sum_f |\langle f | n_q^\dagger | 0 \rangle|^2 \delta(\omega - \epsilon_f + \epsilon_0) \quad (2)$$

in the thermodynamic limit  $L \rightarrow \infty$  taken at a constant filling factor  $\nu = N/L \leq 1/2$ . In Eq. (2),  $n_q^\dagger = \sum_k \psi_k^\dagger \psi_{k-q}$  with  $\psi_k = L^{-1/2} \sum_m e^{-imk} \psi_m$ ,  $|f\rangle$  is an eigenstate of Eq. (1) with energy  $\epsilon_f$ , and  $|0\rangle$  is the ground state with  $\epsilon_0$  being the ground state energy.

In any 1D system, conservation laws restrict the support of correlation functions in  $(\omega, q)$  plane. For example,  $S(q, \omega) > 0$  only at  $\omega > \omega_0(q)$ , see Fig. 1. On general grounds,  $S(q, \omega)$  is expected to exhibit a power-law singularity at the threshold [6],

$$S(q, \omega) \propto [\omega - \omega_0(q)]^{-\mu}. \quad (3)$$

Although exact eigenstates of integrable models can be constructed using the Bethe ansatz [2], evaluation of dynamic correlation functions is very difficult. A considerable progress was achieved in understanding *gapped* models [7]. However, it is still largely an open problem in the *gapless* case, and, with few exceptions (see, e.g., [8, 9, 10, 11]), the threshold exponents  $\mu$  are not

known. For the model (1), the most complete results so far were obtained by combining numerics with the algebraic Bethe ansatz [12, 13]. The main limitation of this technique is very slow convergence towards the thermodynamic limit, which makes it very difficult to evaluate the exponent.

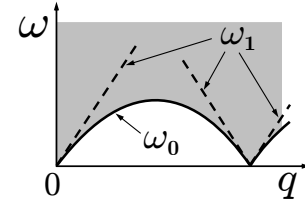


FIG. 1: Support of the structure factor in  $(\omega, q)$  plane. For  $q \neq 0, 2k_F$ , the boundary of the support  $\omega_0(q)$  lies below the straight dashed lines  $\omega_1(q) = \min\{vq, v|q - 2k_F|\}$ ; here  $k_F = \pi\nu$  is the Fermi momentum.

In the alternative Luttinger liquid approach [1, 3, 14], a 1D system is described by two parameters, the sound velocity  $v = (d\omega_0/dq)_{q \rightarrow 0}$ , and the Luttinger parameter  $\kappa$  characterizing the interaction strength. At  $q \rightarrow 2k_F$ , Luttinger liquid theory yields Eq. (3) with the exponent

$$\mu_L = 1 - \kappa. \quad (4)$$

At  $q \rightarrow 0$ , however, one finds  $S \propto \delta(\omega - vq)$ . The discrepancy with Eq. (3) is due to the omission in the fixed-point Luttinger liquid Hamiltonian [3, 14] of the irrelevant in the RG sense operators [13, 14] representing the spectrum nonlinearity. Indeed, for small  $q$ , most of the spectral weight of  $S(q, \omega)$  is confined to a narrow interval of  $\omega$  of the width  $\delta\omega \sim \omega_1 - \omega_0$  about  $\omega = \omega_1$ , while Eq. (3) is applicable at  $\omega - \omega_0 \ll \delta\omega$  [6]. For a linear spectrum  $\delta\omega = 0$ , which makes the regime of Eq. (3) inaccessible. For the same reason, the Luttinger liquid result (4) is valid, strictly speaking, only at  $\omega - \omega_0 \gg \delta\omega$ , and the exact exponent may differ from  $\mu_L$ .

In fact, the true threshold exponents often deviate from the Luttinger liquid theory predictions already in the lowest order in the interaction strength [15]; for  $S(q, \omega)$  near  $q = 2k_F$ , such deviations show up at  $q > 2k_F$ .

In this Letter we develop a technique that allows exact evaluation of the exponents characterizing threshold singularities. The technique is applicable to any correlation function that exhibits a threshold behavior and to any gapless model integrable by the Bethe ansatz. We illustrate the idea of the method by working out the dynamic structure factor (2) for the model (1) as an example.

Among various states  $|f\rangle$  for which  $\langle f|n_q^\dagger|0\rangle \neq 0$  [see Eq. (2)] for a given  $q$ , one state, say,  $|f_q\rangle$ , has the lowest energy  $\epsilon_q = \epsilon_0 + \omega_0(q)$ . Consider now a *deformed* Hamiltonian  $\tilde{H}$  with the following properties:

- (i) The deformed Hamiltonian  $\tilde{H}$  is local.
- (ii)  $\tilde{H}$  commutes with  $H$ , so that  $H$  and  $\tilde{H}$  have the same set of eigenstates  $|f\rangle$ .
- (iii) The states  $|0\rangle$  and  $|f_q\rangle$  represent the doubly-degenerate ground state of  $\tilde{H}$ .
- (iv) The deformation  $H \rightarrow \tilde{H}$  is *continuous* in the sense that if the state  $|f\rangle$  has momentum  $q$  and its energy  $\epsilon_f$  is close to  $\epsilon_q$ , then the corresponding eigenvalues of  $\tilde{H}$  satisfy  $\tilde{\epsilon}_f - \tilde{\epsilon}_q = \epsilon_f - \epsilon_q + O[(\epsilon_f - \epsilon_q)^2]$ ; similarly,  $\tilde{\epsilon}_f - \tilde{\epsilon}_0 = \epsilon_f - \epsilon_0 + O[(\epsilon_f - \epsilon_0)^2]$  for states  $|f\rangle$  with zero momentum.

Once the Hamiltonian  $\tilde{H}$  satisfying these conditions has been constructed, it can be analysed using conventional field-theoretical methods [3]. In particular, condition (i) allows one to identify the low-energy projections of microscopic fields with local operators in the effective continuum description. The coupling constants of this effective low-energy theory can be found by comparing its low-energy spectrum with that of  $\tilde{H}$ . (Essentially the same ideas are behind the Luttinger liquid description of the low-energy excitations of spin chains [3]). Finally, conditions (ii)-(iv) guarantee that the structure factor calculated for the Hamiltonian  $\tilde{H}$  will have a power-law singularity at  $\omega \rightarrow 0$  with the same exponent  $\mu$  that characterizes the threshold behavior in the original model.

Integrable models have an infinite number of independent *local* operators  $I_n$  commuting with  $H$  (integrals of motion). Thus, any Hamiltonian of the form

$$\tilde{H} = \sum c_n I_n \quad (5)$$

will satisfy conditions (i) and (ii).

For free fermions  $|f_q\rangle = \psi_{k_F}^\dagger \psi_{k_F-q} |0\rangle$ , see Fig. 2(a), and the integrals of motion have a simple form. Conditions (ii)-(iv) will be fulfilled if the single-particle spectrum of the deformed Hamiltonian has the shape sketched in Fig. 2(b). While this is not sufficient to determine the coefficients  $c_n$  uniquely, the low-energy spectrum of  $\tilde{H}$  is completely specified.

In the Bethe ansatz, excitations of integrable models such as Eq. (1) are classified in terms of fermion-like quasiparticles and quasiholes [2]. Similar to free

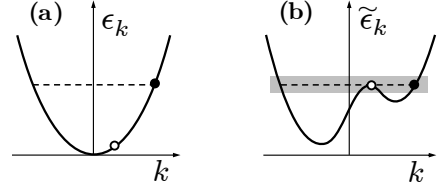


FIG. 2: (a) For free fermions ( $\Delta = 0$ ) and for  $\nu < 1/2$  and  $q < 2k_F$ , the state  $|f_q\rangle$  consists of a single particle-hole pair added to the Fermi sea: the particle is created at the Fermi momentum  $k = k_F$ , and the hole at  $k = k_F - q$ . (b) Single-particle spectrum of the deformed Hamiltonian  $\tilde{H}$ : only states in a narrow strip of energies (shaded) about the Fermi level (dashed line) contribute to the structure factor near the threshold.

fermions, the state  $|f_q\rangle$  corresponds to a quasiparticle with momentum  $k_F$  and a quasihole with momentum  $k_F - q$  added to the ground state, cf. Fig. 2(a).

Provided that the quasiparticle spectrum of the deformed Hamiltonian (see below) is similar to that shown in Fig. 2(b), it is obvious that the infrared fixed point of  $\tilde{H}$  corresponds to a single hole minimally coupled to the right- and left-moving fermions with linear spectrum. We introduce bosonic fields  $\varphi_\pm$  which satisfy  $[\varphi_\alpha(x), \varphi_{\alpha'}(y)] = i\pi\alpha\delta_{\alpha,\alpha'} \text{sgn}(x - y)$ , and the field  $d$  which describes an infinitely heavy hole [16]. The fixed-point Hamiltonian then assumes the form familiar from the x-ray edge singularity problem [17],

$$\tilde{H} = \int \frac{dx}{4\pi} \sum_\alpha v_\alpha \left[ (\partial_x \varphi_\alpha)^2 - 2\beta_\alpha (\partial_x \varphi_\alpha) d(x) d^\dagger(x) \right]. \quad (6)$$

The low-energy projection of the microscopic field  $\psi_m$  is given by  $\psi_m = \sum_\alpha e^{i\alpha k_F x} \psi_\alpha(x) + e^{i(k_F - q)x} d(x)$ , where  $m = x$  is treated as a continuous variable and the fields  $\psi_\pm$  are related to  $\varphi_\pm$  according to

$$\psi_\alpha \propto \exp[i\alpha(\varphi_\alpha \cosh \vartheta - \varphi_{-\alpha} \sinh \vartheta)], \quad e^{-2\vartheta} = \kappa. \quad (7)$$

The leading contribution to the density operator  $n_q^\dagger$  [see Eq. (2)] is then given by

$$n_q^\dagger \propto \int dx \psi_+^\dagger(x) d(x). \quad (8)$$

Evaluation of the structure factor (2) using Eqs. (6)-(8) yields a power-law singularity with the exponent

$$\mu = 1 - \left( \cosh \vartheta + \frac{\beta_+}{2\pi} \right)^2 - \left( \sinh \vartheta + \frac{\beta_-}{2\pi} \right)^2. \quad (9)$$

We now sketch the construction of the deformed Hamiltonian (5) and the derivation of the coupling constants of the corresponding fixed-point Hamiltonian (6). We choose  $I_0 = \sum_m \psi_m^\dagger \psi_m$ , so that  $c_0$  in Eq. (5) plays the role of the chemical potential. For  $n > 0$ , the integrals of motion are expressed via the derivatives of the

transfer matrix (trace of the monodromy matrix)  $\tau(\xi)$  with respect to the spectral parameter  $\xi$  [2],

$$I_{n>0} = i \left[ d^n \ln \tau / d\xi^n \right]_{\xi \rightarrow i\pi/2 - i\eta}. \quad (10)$$

The first operator in this hierarchy is proportional to the Hamiltonian itself:  $I_1 = H / \sin(2\eta)$ . The next one,  $I_2$ , is given in a closed form in [18].

Consider a quasiparticle (quasihole) excitation of the Hamiltonian (1) characterized by the rapidity  $\lambda$  [19]. By construction, such excitation is an eigenstate of the deformed Hamiltonian  $\tilde{H}$ , see Eq. (5). Using properties of the transfer matrix [2], one can show [20] that the corresponding eigenvalue  $\tilde{\epsilon}(\lambda)$  satisfies the equation

$$\tilde{\epsilon}(\lambda) - \frac{1}{2\pi} \int_{-\lambda_F}^{\lambda_F} d\mu K(\lambda - \mu) \tilde{\epsilon}(\mu) = c_0 + \sum_{n>0} c_n (-1)^n \frac{d^n p_0}{d\lambda^n}. \quad (11)$$

Here the Fermi rapidity  $\lambda_F$  is the solution to  $k(\lambda_F) = k_F$  [19],  $K(\lambda) = d\theta/d\lambda$  where  $\theta(\lambda)$  is the bare two-particle phase shift, and  $p_0(\lambda)$  is the bare particle momentum; for the model (1) these are given by [2]

$$\theta = i \ln \left[ \frac{\sinh(\lambda + 2i\eta)}{\sinh(-\lambda + 2i\eta)} \right], \quad p_0 = i \ln \left[ \frac{\cosh(\lambda - i\eta)}{\cosh(\lambda + i\eta)} \right]. \quad (12)$$

In order to satisfy the conditions (ii)-(iv) above, we impose additional constraints on  $\tilde{\epsilon}(\lambda)$ ,

$$\begin{aligned} \tilde{\epsilon}(\lambda_q) &= \tilde{\epsilon}(\pm \lambda_F) = 0, \quad (d\tilde{\epsilon}/d\lambda)_{\lambda_q} = 0, \\ (d\tilde{\epsilon}/d\lambda)_{\pm \lambda_F} &= (d\epsilon/d\lambda)_{\pm \lambda_F} - \frac{\rho(\lambda_F)}{\rho(\lambda_q)} (d\epsilon/d\lambda)_{\lambda_q}, \end{aligned} \quad (13)$$

where  $\lambda_q$  is the solution to  $k(\lambda_q) = k_F - q$  [19]. The constraints are equivalent to five *linear* equations on the coefficients  $c_n$  in Eqs. (5) and (11). In order to satisfy these equations, it is sufficient to keep the first five integrals of motion in Eq. (5).

The coupling constants of the effective fixed-point Hamiltonian (6) follow from the comparison of the finite-size spectrum of (6) with the exact low-energy spectrum of the deformed Hamiltonian  $\tilde{H}$ . This procedure is standard [2] and yields [20]

$$\beta_{\pm} = \pm 2\pi F(\pm \lambda_F | \lambda_q), \quad (14)$$

where  $F$  is the dressed phase shift that satisfies [2]

$$F(\lambda|\zeta) - \frac{1}{2\pi} \int_{-\lambda_F}^{\lambda_F} d\mu K(\lambda - \mu) F(\mu|\zeta) = \frac{1}{2\pi} \theta(\lambda - \zeta). \quad (15)$$

Eqs. (14) and (15) uniquely define the parameters  $\beta_{\pm}$ , and, therefore, the exponent (9).

Note that  $\beta_{\pm}$  do not depend explicitly on the coefficients  $c_n$ . Indeed, the constraints (13) do not completely fix  $\tilde{H}$  but only specify its low-energy spectrum. We emphasize that our construction does not rely on the model-specific Eq. (12) but is applicable to any model integrable by the algebraic Bethe ansatz.

We now use Eqs. (9), (14), and (15) to evaluate the threshold exponent for the model (1). Precisely at half-filling  $\lambda_F \rightarrow \infty$  [2] and Eq. (15) is solved by Fourier transform with the result

$$F(\pm \infty | \zeta) = \pm (\kappa - 1)/2, \quad (16)$$

where we used the well-known [2] value of the Luttinger parameter at half-filling,  $\kappa = \pi/4\eta$  [4]. Eqs. (9), (14), and (16) then yield a momentum-independent exponent

$$\mu_0 = \frac{1 - \kappa}{2} \left( \kappa - \frac{1}{\kappa} + \frac{2}{\sqrt{\kappa}} \right), \quad \nu = 1/2. \quad (17)$$

Comparison with Eq. (4) shows that the exact exponent  $\mu_0$  is *smaller* than the Luttinger liquid result  $\mu_L$  (note that  $\kappa$  varies between 1/2 and 1). For a weak interaction,  $\mu_L - \mu_0 \approx \mu_L^2/2 \approx 2(\Delta/\pi)^2$ .

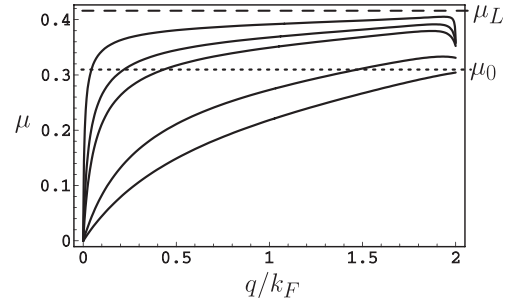


FIG. 3: Threshold exponent  $\mu(q)$  for  $\Delta = 0.9$  and for  $\nu = 0.4, 0.45, 0.49, 0.495, 0.499$  (bottom to top). The dashed horizontal lines correspond to  $\mu_L$  and  $\mu_0$  at half-filling.

Away from half-filling, Eq. (15) can be solved numerically. The resulting exponent is  $q$ -dependent, see Fig. 3. It varies from  $\mu(0) = 0$  to  $\mu(2k_F) = \mu_2$  with  $\mu_0 < \mu_2 < \mu_L$ ; the exact value of  $\mu_2$  depends on both  $\Delta$  and  $\nu$  [20]. Very close to half-filling, the dependence  $\mu(q)$  is nonmonotonic: outside narrow intervals of the width

$$\delta k \sim 1/2 - \nu \ll k_F \quad (18)$$

near  $q = 0$  and  $q = 2k_F$ , the exponent approaches a constant,  $\mu(q) \approx \mu_1 = \text{const}$ . Surprisingly,  $\mu_1$  coincides with the Luttinger liquid exponent  $\mu_L$  rather than with the exact half-filling result  $\mu_0$ .

This discrepancy originates in the peculiar behavior of the phase shifts near the Fermi points. Consider Eq. (15) at  $|\zeta \pm \lambda_F| \gg \delta\lambda$  with  $\delta\lambda = 1 - 2\eta/\pi$  (this limit corresponds to  $q$  away from  $q = 0, 2k_F$ ). In order to find the phase shift  $F(\lambda|\zeta)$  for  $\lambda_F \gg \delta\lambda$  (i.e., close to half-filling) and  $\lambda \approx \lambda_F$  (i.e., close to the right Fermi point), we replace  $\theta(\lambda - \zeta)$  in the r.h.s of (15) by  $\theta(\infty)$ , and extend the integration in the l.h.s. to  $-\infty$ . The resulting equation

$$F(\lambda|\zeta) - \frac{1}{2\pi} \int_{-\infty}^{\lambda_F} d\mu K(\lambda - \mu) F(\mu|\zeta) = \frac{1}{2\pi} \theta(\infty), \quad (19)$$

as well as the similar equation for  $\lambda \approx -\lambda_F$ , describes the fractional charge function [2]. Its solution yields

$$2\pi F(\lambda|\zeta) = \begin{cases} \gamma_0, & \lambda, \lambda_F - \lambda \gg \delta\lambda \\ \gamma_1, & \lambda_F - \lambda \ll \delta\lambda \end{cases} \quad (20)$$

with  $\gamma_0 = \pi(\kappa - 1)$  and  $\gamma_1 = \pi(\kappa - 1)\kappa^{-1/2}$ . In other words, the limits  $\lambda \rightarrow \pm\lambda_F$  and  $\lambda_F \rightarrow \infty$  for the phase shift  $F(\lambda|\zeta)$  do not commute. If the limit  $\lambda \rightarrow \pm\lambda_F$  is taken first, and the resulting phase shifts are substituted into Eq. (14), one finds  $\beta_{\pm} = \gamma_1$ . Eq. (9) then yields  $\mu_1 = \mu_L$ . However, by taking first the limit  $\lambda_F \rightarrow \infty$  (i.e.,  $\nu \rightarrow 1/2$ ), one would find  $\beta_{\pm} = \gamma_0$  and  $\mu_1 = \mu_0$ .

The noncommutativity of limits has observable consequences. Indeed,  $F(\lambda|\zeta)$  characterizes the strength of the interaction between a quasihole at rapidity  $\zeta$  and a quasiparticle at rapidity  $\lambda$ . According to Eq. (20), the phase shift at  $\lambda \approx \pm\lambda_F$  changes with  $\lambda$  on the scale  $\delta\lambda \ll \lambda_F$ . In the momentum space, this corresponds to narrow intervals of the width  $\delta k = 2\pi\rho(\lambda_F)\delta\lambda \sim (1/2 - \nu)$  near  $k = \pm k_F$  (here we used the well-known [2] result for  $\rho(\lambda)$  near half-filling). States within or outside these intervals interact with the quasihole with coupling constants  $\beta_{\pm} \approx \gamma_1$  or  $\beta_{\pm} \approx \gamma_0$ , respectively.

As the filling factor approaches  $1/2$ , the interval  $\delta k$  collapses. For a finite-size system close to half-filling,  $\delta k$  will eventually become compatible with the momentum quantum  $\sim 1/L$ . In this limit, the threshold behavior is dominated by states outside the interval  $\delta k$ . Accordingly, the exponent  $\mu_1$  that characterizes the threshold singularity away from  $q = 0, 2k_F$  exhibits a crossover from  $\mu_1 = \mu_L$  at  $1 \gg \delta k \gg 1/L$  to  $\mu_1 = \mu_0$  at  $\delta k \ll 1/L$ .

In the recent study [21] the exponent  $\mu$  at half-filling was found to be equal to  $\mu_L$ . Our consideration shows that  $\mu$  indeed approaches this value when  $\nu \rightarrow 1/2$ . However, because the limits  $\nu \rightarrow 1/2$  and  $\omega \rightarrow \omega_0$  do not commute, the region of applicability of the result  $\mu = \mu_L$  is limited to  $\omega - \omega_0 \ll \nu\delta k$ . Precisely at half-filling  $\delta k = 0$ , and the exponent is given by Eq. (17) instead.

It should be mentioned that the two-spinon contribution to the structure factor has a square-root singularity at  $\omega \rightarrow \omega_0$  [22]. This result was obtained by approaching  $\Delta = 1$  from the *gapful* side of the transition  $\Delta > 1$ . We found  $\mu_0 < 1/2$  in the *gapless* regime  $\Delta < 1$ , see Eq. (17) above. The discrepancy suggests that the threshold exponent  $\mu_0(\Delta)$  has a discontinuity at  $\Delta = 1$ .

Finally, for  $\delta k > 0$  and when  $q$  approaches either  $0$  or  $2k_F$ , the situation is complicated by the competition between two small energy scales,  $\nu\delta k$  and  $\delta\omega$  (see above). The behavior of the structure factor in this regime will be discussed in details elsewhere [20]. At small  $q$ , it agrees with the first-order result of [6]:  $\mu(q) \sim (\Delta/\delta k)q$  for  $0 < \delta k \ll 1$  and  $\mu_0 \approx \mu_L \sim \Delta$  for  $\delta k = 0$ ; the two exponents merge at  $q \sim \delta k$ .

To conclude, we proposed a method of evaluating the

exponents characterizing threshold singularities in the dynamic response functions of gapless integrable models. Application of the method to the dynamic structure factor of 1D spinless fermions on a lattice revealed unexpected complexity in the dependence of the threshold exponent on the system parameters near half-filling.

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